

The Electron Range and the Backscattering Coefficients in Compound Semiconductors: Comment on Z.Rouabah, A. Bouzid, C. Champion, N. Bouarissa [Sol.Stat.Comm. 151 (2011) 838]

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Abstract

This work is a comment on the paper of Z.Rouabah et al [Sol.Stat.Comm. 151 (2011) 838]. Indeed, it is shown that the transport cross-section used in their work is inaccurate and really not based on Jablonski model [Phys. Rev. B 58 (1998) 16470] as well. Moreover, it is noted that their calculation method concerning the compound materials is not explained also not justified. Moreover, some recommendations have been indicated on the use of a given model (developed initially for a monatomic solid target) to study the compound material which is not respected in the case of the above mentioned paper. In addition, it is shown that all their results concerning GaN, GaAs and InSb semiconductor materials must be reviewed.

Keywords

Semiconductors; Low-energy Electron; Electron Backscattering; Electron Range; Monte Carlo Simulation

Introduction

Electron material interaction is tied much importance to many domains of analytical techniques such as electron probe microanalysis, Auger electron spectroscopy, scanning electron microscopy (SEM) etc (Bentabet^a et al. 2013, Bentabet et al. 2010). Two transport quantities play a great role in the majority of such mentioned studies: the backscattering coefficient (BSC) and the range of penetration (R). For example, the BSC is a major factor to validate the model used in the

simulation and to inform about the absorbed rate of incident particles (Bentabet 2011). Indeed, by this work, some comments are presented, about a paper of (Rouabah et al. 2011) studying the electron transport in GaN, GaAs and InSb semiconductor targets using analytical models. These materials are base of a number of electronic devices, as the authors of (Rouabah et al. 2011) said "The choice of target materials is based on their importance for many applications in semiconductor technology... As for GaAs, it is the most technologically important material for device applications. Concerning GaN, interest on this material has grown since it has successful applications in blue lasers and light emitting diodes. It has also applications in high-frequency optoelectronics and at high temperatures". Besides, the indium antimonide (InSb) is a semiconductor consisting of III-V compounds of antimony and indium. It has a narrow gap used particularly as infrared detector, in thermal imaging, in infrared homing guidance systems and infrared astronomy. Detectors, based on indium antimonide, are sensitive to wavelengths between 1 and 5 μm . So, for such reasons, the authors (Rouabah et al. 2011) took these materials as targets for electron beam to carry out their study.

In this paper, our work is divided into two parts: the first one represents generalities on two great axes: the first of which shows the electronic properties of the above

mentioned materials near or in the thermodynamic equilibrium, while the second shows the electron beam transport in these materials (i.e. the incidental electron is outside the thermodynamic equilibrium with the target). However, the second part represents our commentary on the work of (Rouabah et al. 2011) which is part of the second axis.

The Electronic Interaction in GaN, GaAs and InSb Semi Conductors

The Electronic Properties of GaN, GaAs and InSb

GaN, GaAs and InSb semi conductors have been studied using the first-principle total-energy calculations based on the density functional theory using the pseudopotential method, and a plane-wave expansion of the wave functions as implemented in the ABINIT code.

The exchange and correlation energy is treated using the local density approximation (LDA) with the Ceperley–Alder form (1980) as parameterized by Perdew and Zunger (1981). The interaction of the valence electrons with the ionic cores is represented by separable, norm-conserving Troullier–Martins pseudo-potentials (1991).

The pseudo-potentials were generated using Hartwigsen–Goedecker–Hutter scheme (www.abinit.org). A basis of plane waves up to a kinetic energy of 80 Hartree was used. Reciprocal space integration was performed by k-points sampling with sets of special points of $8 \times 8 \times 8$ obtained using the standard special k point technique of the Monkhorst and Pack (1976).

The zinc-blende GaX (X=N and As) and InSb have a cubic symmetry belonging to the F-43M (space group $N^{\circ}216$). The Ga (or In) atom is located at 4a (0, 0, 0) site and the X (or Sb) atom is located at 4c (1/4, 1/4, 1/4) site (Bouhadda et al. 2012). The calculated equilibrium lattice constant for zinc-blend GaN, GaAs and InSb from LDA, compared to the experimental data are presented in Table 1. Our calculated lattice parameters seem very close to the experimental one (Madelung 1982, Lie et al. 1992, Straumanis et al. 1965).

TABLE 1 THE CALCULATED AND EXPERIMENTAL LATTICE PARAMETERS (IN Å) OF THE ZINC-BLENDE GAN, GAAS AND INSb.

	GaN	GaAs	InSb
This work	4.335	5.531	6.35
Exp.	4.50 ^a	5.650 ^b	6.479 ^c

^a Madelung 1982, ^b Lie et al. 1992, ^c Straumanis et al. 1965

Elsewhere, the importance of GaN, GaAs and InSb materials could be validated by their electronic properties.

The figures (1-3) represent the band structure of the above compound materials respectively. Indeed, it is remarked that all these materials have a direct band gap. Consequently, the transition from the valence band to the conduction one could be done by energy absorption phenomena without the phonon contribution. Moreover, the semi conductor group compounds (GaN, GaAs and InSb) shows three typical gaps (large, medium and tight) respectively. Each category of these later plays an important role in the technology application.

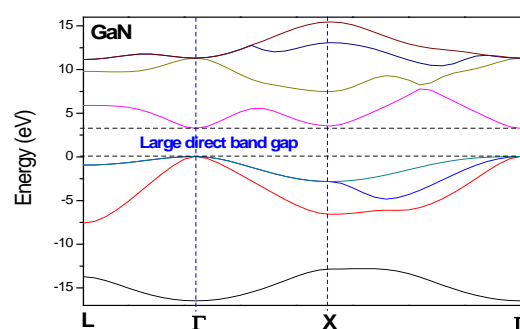


FIG. 1 BAND STRUCTURES OF GaN.

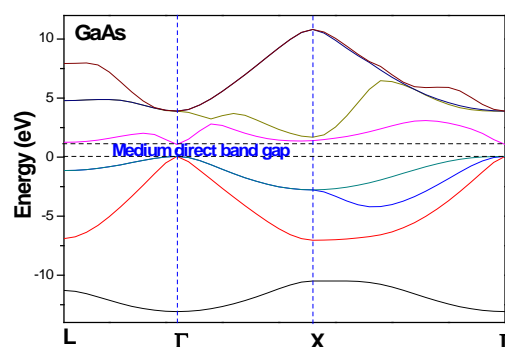


FIG. 2 BAND STRUCTURES OF GaAs.

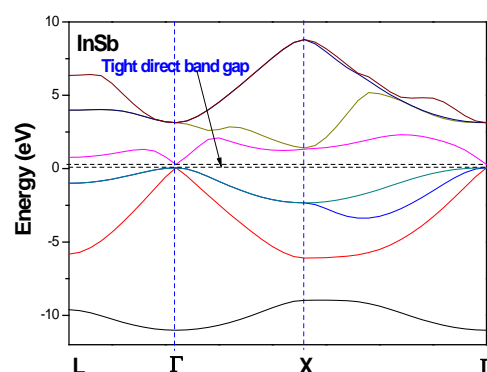


FIG. 3 BAND STRUCTURES OF InSb.

The Electron Beam Transport in GaN, GaAs and InSb Targets

Generally the solid targets are presented in the form of thick or thin films attacked by slow electrons. In other words, it is supposed that the target is taken as a

parallelepiped with infinite length and width and thickness (half entire space). The coordinates of the particles are located using a (OXYZ) reference so that axis (OX) and (OY) belong to the exterior surface outside of the target (entry surface) and (OZ) is directed toward the interior of the solid (Bentabet et al. 2009). The angles θ and φ represent the polar and the azimuthal angles which can be varied as follow: $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$ (Bentabet 2012) (see figure 4). A number of methods could be used to follow the electron trajectory in the solid target since its entry in the target to its final stage which is defined as either the backscattering or the absorption phenomena. In the figure (2) we present a Monte Carlo scheme used by number of authors.

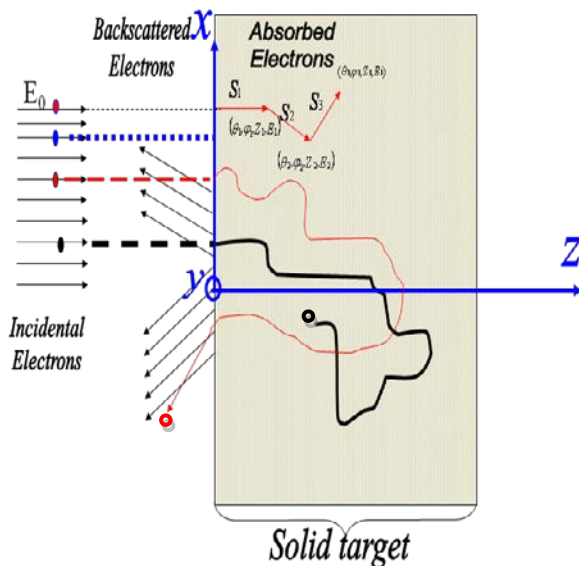


FIG. 4 THE SLOW ELECTRON TRANSPORT SCHEME IN THE INTERIOR OF THE SOLID TARGET. S_i : THE DISTANCE BETWEEN TWO SUCCESSIVE COLLISIONS (i INDICATES THE COLLISION NUMBER, $i=1, 2, \dots$). Z_i : THE NORMAL DISTANCE BETWEEN THE ENTRY SURFACE AND THE ELECTRON. θ_i AND φ_i ARE THE AZIMUTAL AND SCATTERING ANGLES. E_i THE ELECTRON ENERGY AFTER COLLISION. THE RED TRAJECTORY IS OF THE BACKSCATTERED ELECTRON. THE BLACK TRAJECTORY IS OF THE ABSORBED ELECTRON.

Both the two phenomena could be defined as follows:

- An electron is absorbed if its energy is lost during the different inelastic processes with the solid target, from its initial energy until it arrives at the thermal equilibrium with the medium (the bold black trajectory in figure (4)). In the absorption phenomena, number of quantities could describe the absorption of the electron; among them the range of penetration which is defined as the path length travelled by a particle (in an infinite medium) before being absorbed (Salvat et al. 2003). In other words, R is the average track length of absorbed particles

(Penelope nomination).

- An electron considered as backscattered if, after interaction with the solid target, this electron leaves the solid by the entry surface (the red trajectory in figure (4)). Under these conditions, the backscattered electrons are those which have energy higher than the thermal energy rather higher than the surface energy and its coordinate (Z) is lower than zero. Several quantities could describe this category of transport phenomena, in particular, the backscattering coefficient (BSC). BSC is the backscattering probability which is the ratio of the backscattered particles to the incidental ones.

Comments on the Paper of Rouabah et al. (2011)

According to Rouabah et al. (2011), they calculated the backscattering coefficient (BSC) using the Vicanek and Urbassek (1991) formula. Hence, they used four models to calculate the range and one model to calculate the transport cross-section (TCS) as well. Moreover, they think that their results concerning some semi-conductors seems to be seen as the first predictions for low-energy electron BSC.

Carefully analyzing (Rouabah et al. 2011) paper, an anomalous problem is noted and consequently the results must be reviewed and corrected.

The Jablonski Transport Cross Section

Rouabah et al (2011) attributed an old TCS to Jablonski (1998) and they said in their abstract (Rouabah et al. 2011) in the next paragraph: "The cross-sections used to describe the electron transport are determined via the appropriate analytical expression given by Jablonski (1998) whose new improved version has been recently reported by Rouabah et al (2009)". Unfortunately, this information is inaccurate. Actually, their work "Rouabah et al. 2011" is based on the TCS obtained by integrating a screened cross-section. Knowing that this latter is obtained by applying the first order Born approximation on a screened potential (Jablonski 1998, Bentabet^a et al. 2013).

So, the TCS obtained by integrating the screened cross section is given by (Bentabet^a et al. 2013):

$$\sigma_{tr}^B = \frac{32\pi Z^{2/3} C_F^4 a_0^2}{(\mu^\infty)^4} \frac{1}{\epsilon_0^2} \left[\ln(1 + \epsilon_0) - \frac{\epsilon_0}{1 + \epsilon_0} \right] \quad (1)$$

With,

$$C_F=0.8853414, \varepsilon_0 = 0.230440 \frac{E}{(\mu^\infty)^2 Z^{2/3}}, \mu^\infty = 1.22.$$

where σ_{Tr}^B , Z and E are the transport cross-section, the atomic number of the atom target and the electron energy, respectively.

We note that we have shown step by step in our recent paper (Bentabet^a et al. 2013) that the age of σ_{Tr}^B is more than 60 years old (since the works of Wentzel (1927) and Nigam (1959)). Moreover, it is worth noting that the first order Born approximation fails at lower energies (Jablonski 1998, Bentabet^a et al. 2013), and the σ_{Tr}^B standard deviation reaches hundreds percent for number of elements compared to that obtained by quantum methods. For example the σ_{Tr}^B deviation reaches ~1500% for Au at $E = 250$ eV (which is the proof that Jablonski cannot propose such model with such unacceptable deviation) whereas the authors of (Rouabah et al. 2009, Rouabah et al 2011) attributed eq. (1) to Jablonski.

Actually, the TCS proposed by Jablonski lies in his paper (Jablonski 1998): "To obtain a more accurate analytical expression for σ_{Tr} , we need an additional analytical function $G(\varepsilon_0)$ correcting σ_{Tr}^B

$$\sigma_{Tr} = \sigma_{Tr}^B G(\varepsilon_0) \quad (2)$$

With

$$G(\varepsilon_0) = \varepsilon_0 \exp \left\{ \sum_{i=1}^4 A_i \left[\ln(10\varepsilon_0) \right]^{i/2} \right\} \quad (3)$$

where A_0, A_1, A_2, A_3 , and A_4 are fitted constants for each element." Therefore the Jablonski transport cross section is that given by (2-3) which correspond to Eqs. (21) and (22) of (Jablonski 1998).

Consequently, the next two paragraphs of (Rouabah et al 2011) must be reviewed:

- In their abstract: "The cross-sections used to describe the electron transport are determined via the appropriate analytical expression given by Jablonski [A. Jablonski, Phys. Rev. B 58(1998) 16470] whose new improved version has been recently reported by Rouabah et al. [Z. Rouabah, N. Bouarissa, C. Champion, N. Bouaouadja, Appl. Surf. Sci. 255 (2009) 6217]."
- In their section 3: "The electron transport cross-sections have been calculated by using the new improved expression suggested by Rouabah et al. of the approximate analytical one previously derived by Jablonski."

Comment on the Accuracy of the Used Transport Cross Section in Rouabah et al. 2011

Rouabah et al (2011) used the TCS proposed by (Rouabah et al. 2009). However, before quoting our overview points, we recall that Rouabah et al (2009) used the same transport cross section expressed by equation (1) where the only difference is that μ^∞ has been taken as a free parameter. Thus, to determine μ^∞ , σ_{Tr}^B has been adjusted to Mayol et al TCS (1997). After a fitting process, they suggested the next interpolation form of μ^∞ given by:

$$\mu^\infty = 2.17 \times 10^{-7} Z^3 - 1.54 \times 10^{-4} Z^2 + 0.03 Z + 0.89 \quad (4)$$

It is noted that we have shown step by step in our recent paper (Bentabet^a et al. 2013) that Rouabah et al (2009) TCS fit is not accurate (the deviations were as examples: for Au: 96% and 30.3 % at $E=250$ and 500 eV respectively, for Al: 21% and 12 % at $E=250$ and 500 eV... respectively, for Cu: 41%, 20% and 10.2 % at $E=250, 500$ and 1000 eV respectively,).

Calculation Method of Rouabah et al. (2011)

There's a great ambiguity regarding the calculation method of (Rouabah et al. 2011). For example, no one can take again their calculation without knowing in detail the TCS and the ranges used in their work. For example, no explanation has been given about how they calculated the range of Kanaya and Okayama (1972) and the BSC of GaN, GaAs and InSb. This ambiguity is another **inaccuracy** of Rouabah et al (2011) work.

For more details;

The range of Kanaya and Okayama is given by:

$$R_{K-O} = \frac{2.76 \times 10^{-11} A E_b^{5/3} (1 + 0.978 \times 10^{-6} E_b)^{5/3}}{Z^{8/9} \rho (1 + 1.957 \times 10^{-6} E_b)^{4/3}} \quad (6)$$

Where R_{K-O} , A , E_b , ρ are Kanaya and Okayama range, the atomic weight, the electron incidence energy and the density of the target. In terms of question: how did they calculate the atomic weight and the atomic number of GaN, GaAs and InSb?

The Vicanek and Urbassek BSC model: We recall that Rouabah et al. (2011) used Vicanek and Urbassek (1991) model which showed that BSC (denoted η in the following) has been calculated analytically at normal angles of incidence by:

$$\eta = \left(1 + a_1 \frac{1}{v^2} + a_2 \frac{1}{v} + a_3 \frac{1}{v^3} + a_4 \frac{1}{v^2} \right)^{-1/2} \quad (7)$$

$$\text{with: } a_1 = \frac{6}{\sqrt{\pi}}, a_2 = \frac{27}{\pi}, a_3 = \frac{27}{\sqrt{\pi}} \left(\frac{4}{\pi} - 1 \right), a_4 = \left(\frac{3}{2} - \sqrt{2} \right)^{-2}.$$

In expression (7), ν is the mean number of wide angle collisions defined as,

$$\nu = NR\sigma_{tr} \quad (8)$$

With R and σ_{tr} are the range and the transport cross-section and N is the number of atoms per unit of volume in the solid target given by:

$$N = \frac{N_{Av}\rho}{A} \quad (9)$$

with N_{Av} is Avogadro number.

Indeed, to calculate η they have needed to know " ν ". By consequence they have needed to calculate σ_{tr} and A of GaN, GaAs and InSb. Unfortunately, Rouabah et al (2011) have not given any information about the calculation of these quantities!

Is Rouabah et al (2011) Expression "*The results May be Seen as the First Predictions ...*" True?

When said it is reported in the ABSTRACT of Rouabah et al (2011) the next paragraph that "The results may be seen as the first predictions ..." they should be very careful because when someone reading this later will believe, certainly, that the authors of such paragraph will show a new method or a new idea somewhere. However, the authors of (Rouabah et al. 2011) have not explained any method concerning the passage from monatomic materials to compound ones (see above). In addition, Rouabah et al. (2011) did not present any comparison with the experience or with the Monte Carlo simulation concerning the compound materials. Before giving our viewpoint concerning this latter, we recall that number of Monte Carlo codes have been developed to study simple and complex systems (medicals, nuclear, materials, etc.). Among "the simplest systems" is that studied by (Rouabah et al. 2011) (the simplest geometry of the incidental particles source and the simplest geometry of the target).

For example, Penelope (Salvat et al. 2003) is an accurate Monte Carlo code developed since about twenty years.

In Penelope manual (version 2008) we found in page 3 the next expression:

---- MATERIAL DATA FILE ----

PENELOPE reads the required information about each material ... To simulate geometrical structures with several materials, .. PENELOPE labels the M-th material in this file with the index MAT=M... The maximum number of different materials that PENELOPE can handle simultaneously is fixed by the parameter MAXMAT, which in the present version is

set equal to 10."

Thus, the use of Penelope code straightforwardly allows the calculation of the backscattering coefficient and the range of GaN, GaAs and InSb with reasonable results.

We think that this claim "the results may be seen as the first time" is quite similar to the following example:

One would like to calculate for example $(1.0201030406)^{1/3}$. May be, no person has calculated this equation previously. So, anyone could claim "the result $(1.0201030406)^{1/3} = 1.00665660482660198750765839$ may be seen as the first time". But, is this claim a scientific fact? Of course no, because, really, anyone who masters the use of the calculator, could calculate this latter " $(1.0201030406)^{1/3}$ " without any difficulties.

Following the same argument. So, when anyone who masters the use of Penelope code, could calculate the BSC and the range of GaN, GaAs, InSb and any binary compound material in short time and without any difficulties. In addition, the important question is: are the BSCs of (Rouabah et al. 2011) true (see below)?

Thus, on the basis that (Rouabah et al. 2011) have not explained their calculation method despite the fact of the possibility to use accurate Monte Carlo codes, the use of such paragraph of Rouabah et al (2011) "*The results may be seen as the first predictions*" is inaccurate.

The Large Deviation of Rouabah et al (2011) Results

It is noted that Rouabah et al. (2011) have repeated an important part (i.e. using the same procedures) of the work of Kurniawan and Ong (2007). In other words, Kurniawan and Ong used three models to calculate the range: Gruen et al (1957) (R_G), Everhart and Hoff (1971) (R_{E-H}) and Kanaya and Okayama (1972) (R_{K-O}). Moreover, Kurniawan and Ong tried to carry out a correction on these ranges by proposing an improvement range (R_{K-O}). However, Rouabah et al. (2011) repeated the same above models to calculate the BSC but without showing any improvement somewhere.

For more details; it is recalled that Kurniawan and Ong used R_{K-O} given by (6) and R_G and R_{E-H} which are given by:

$$R_G = \frac{45.7}{\rho} E_b^{1.75} \quad (10)$$

$$R_{E-H} = \frac{40.}{\rho} E_b^{1.75} \quad (11)$$

It is noted that R_{K-O} can be written as follows:

$$R_{K-O} \approx \frac{2.76 \times 10^{-11} A}{Z^{8/9} \rho} E_b^{5/3} \quad (12)$$

Because $(1 + 0.978 \times 10^{-6} E_b)^{5/3} \times (1 + 1.957 \times 10^{-6} E_b)^{-4/3}$ is a relativistic correction.

Based on the fact that some of the above ranges are semi-empirical models (developed, with a limit validity, on the basis of experimental results) then Kurniawan and Ong proposed an improvement expression given by $R_{Ku-O} = \alpha E_b^\beta$, where α and β are free parameters determined by using the best fit of the ranges obtained by using Monte Carlo code. Hence, they found:

$$R_{Ku-O} = 23.17 E_b^{1.73} \quad \text{for Si} \quad (13)$$

$$R_{Ku-O} = 10.46 E_b^{1.68} \quad \text{for GaN} \quad (14)$$

Consequently, Kurniawan and Ong have suggested an improvement range expression for Si and GaN by by means of Monte Carlo method.

Elsewhere, Rouabah et al (2011) said the next paragraph: *"the proposed range-energy expressions based on the extrapolated range for Si and GaN provided by Kurniawan and Ong at low beam energies."* Unfortunately, this information is inaccurate. The results presented by Rouabah et al (2011) do not correspond to R_{Ku-O} expressions (given by (13-14)). As results, such information needs to be corrected.

To validate the results of Rouabah et al (2011) concerning the compound materials that have been reviewed, it is thought that a similar reasoning of (Kurniawan et al. 2007) can be followed. In other words, their work can be evaluated by carrying out a comparison between the results of Rouabah et al (2011) and those of Penelope code which is an accurate Monte Carlo code (the additively rule and the mean excitation energy have been validated experimentally for compound materials (Barô et al. 1993). Figures (5), (6) and (7) represent the BSCs of Rouabah et al (2011) compared to that of Penelope code. It can be observed is that the deviation between the BSC of GaN (Rouabah et al. 2011) and that of Penelope code is very larger than that in the case of GaAs and InSb (as example the deviation of their BSC by using R_{K-O} is about 55%, 19% and 21% for GaN, GaAs and InSb respectively). This latter allows us to claim that the authors of (Rouabah et al. 2011) have not used the same procedure in the calculation of BSC. Moreover, it is remarked that there is a large deviation between their results and those of Penelope code in all compound materials cases which is the proof of the invalidity of their work, otherwise Penelope is, (as example, too, the deviation of their BSC by using R_{E-H}

is about 75%, 50% and 44% for GaN, GaAs and InSb respectively).

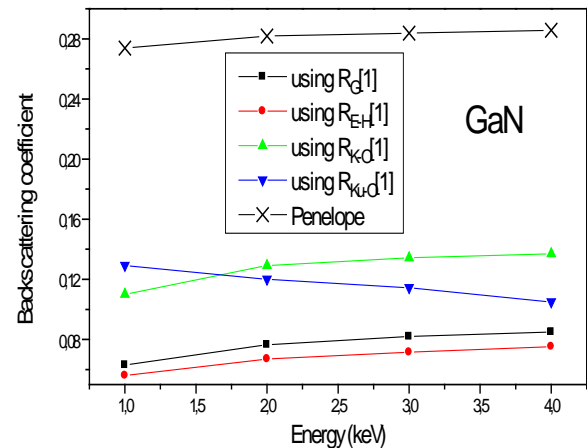


FIG. 5 ELECTRON BACKSCATTERING COEFFICIENT VERSUS ELECTRON PRIMARY ENERGY IN GAN. [1]: ROUBAH ET AL.(2011).

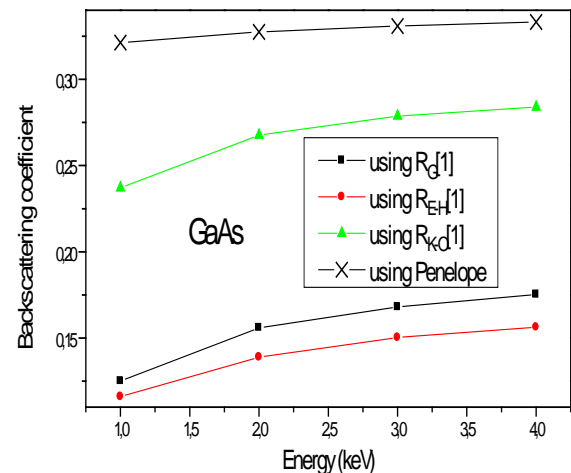


FIG. 6 ELECTRON BACKSCATTERING COEFFICIENT VERSUS ELECTRON PRIMARY ENERGY IN GAAS. [1]: ROUBAH ET AL.(2011).

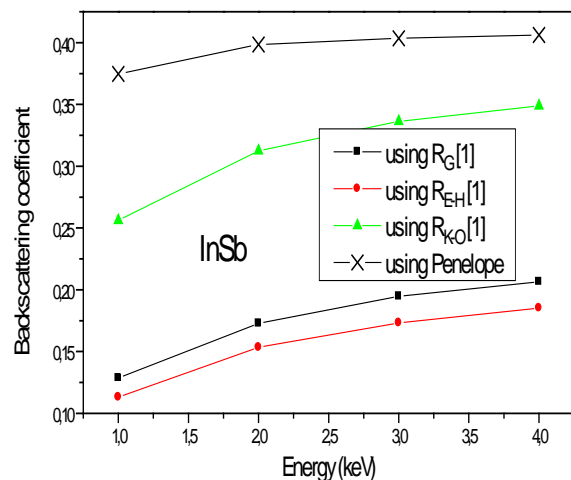


FIG. 7 ELECTRON BACKSCATTERING COEFFICIENT VERSUS ELECTRON PRIMARY ENERGY IN INSB. [1]: ROUBAH ET AL.(2011).

Remark: it is noted that we have tried after a number

of tests (due, unfortunately, to the ambiguity in their calculation) to discover the procedures applied by (Rouabah et al. 2011) to calculate the range and the BSC of compound materials; where it is thought that:

- ✓ Concerning the Kanay and Okayama range: via the reading of Kurniawan and Ong paper (Kurniawan et al. 2007), it is indicated that the authors of (Rouabah et al. 2011) used the next procedure to calculate R_{K-O} :

$$A_{AB} = (A_A + A_B) / 2 \quad (15)$$

$$Z_{AB} = (Z_A + Z_B) / 2 \quad (16)$$

Where A_{AB} and Z_{AB} are the atomic weight and the atomic number of a material up from two elements A and B. For example the atomic number of $Z_{GaN} = (31+7)/2 = 19$. Indeed, we have a reservation about this procedure. It is noted that eqs.(15-16) have been proposed, first, by (Kurniawan et al. 2007). However, the authors (Rouabah et al. 2011) have not cited this latter. This one (i.e. the no citation of the used method especially if they used equations (15-16) proposed first by (Kurniawan et al. 2007)) is another inaccuracy of the work (Rouabah et al. 2011). Secondly, (Kurniawan et al. 2007) adopted equations (15-16) as an intermediate steps (before improvement). Actually, it is totally not a justifiable processing to pass from monatomic materials to compound ones by using the equations (15-16). Moreover, when R_{K-O} given by using equations (6, 15-16) is approximately good for GaN (which has been remarked by (Kurniawan et al. 2007)), it is not recommended to generalize this rule on all R_{K-O} ranges of compound materials because eqs.(15-16) it is a false procedure (except after an agreed R_{K-O} study for number of compound materials).

- ✓ Concerning their BSC results, too, it is reported that the authors (Rouabah et al. 2011) have used the next procedures:

$$\text{For GaN: } \sigma_{tr(GaN)} = (\sigma_{tr(Ga)} + \sigma_{tr(N)}) / 2,$$

$$A_{GaN} = A_{Ga} + A_N = 83.73g \quad (17)$$

$$\text{For GaAs: } \sigma_{tr(GaAs)} = (\sigma_{tr(Ga)} + \sigma_{tr(As)}) / 2,$$

$$A_{GaAs} = (A_{Ga} + A_{As}) / 2 = 72.32g \quad (18)$$

$$\text{For InSb: } \sigma_{tr(InSb)} = (\sigma_{tr(In)} + \sigma_{tr(Sb)}) / 2,$$

$$A_{InSb} = (A_{In} + A_{Sb}) / 2 = 118.285g \quad (19)$$

Equations (17-19) showed that the atomic weight of GaN have been not calculated by

using the same procedure such as on GaAs and InSb.

So, whether the authors of (Rouabah et al. 2011) used these procedures or not, we note that the use of these procedures given approximately the same results presented by (Rouabah et al. 2011).

Conclusion

In summary, it has been shown that Rouabah et al (2011) have applied the Vicanek and Urbassek formula to calculate the backscattering coefficient (BSC) of electrons impinging in GaN, GaAs and InS but without any explanation concerning their method calculation. In addition, it has been also noted that they have used inaccurate transport cross-section model and their BSC results of compound materials have a large deviation with those of Penelope code, as well. Consequently, on the basis that Penelope is an accurate Monte Carlo code, this latter (large deviation results) is the proof that their work is invalid and should be reviewed.

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